The European Synchrotron

Activities EU team

Manuel Sanchez del Rio

OUTLOOK

Historical perspective

- Birth of SHADOW
- First years at ESRF (XOP+SHADOWVUI)
- Upgrade I – Shadow3
- Upgrade II - From SHADOW to Oasys

TOWARDS VIRTUAL EXPERIMENTS: SOFTWARE INTEGRATION (OASYS, ShadowOui)

NEW PROJECTS (HYBRID, DABAM)

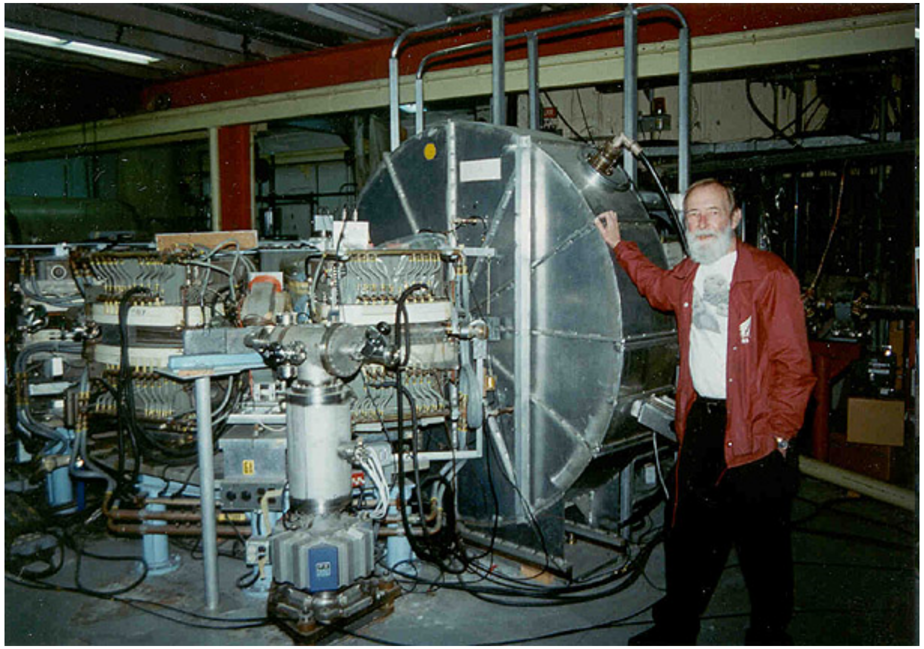
SHADOW3 ACTIVITY

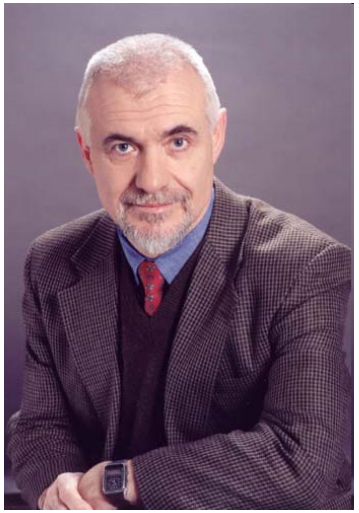
RESEARCH TOPICS

- Partial coherence (Mark)
- Crystal Optics
- Sample scattering – Powder diffraction (Luca)
- Wiggler calculations (Manuel)
- Lenses

BIRTH OF SHADOW - 1984

At the University of Wisconsin during 1965 -1967, a team led by particle physicist Ednor Rowe built *Tantalus*. In 1977 SRC began construction on its own facility focusing on a new and much larger SR source, *Aladdin*.





Scientific motivation:
Grating monochromator design, TGM, ERG, toridal, spherical mirrors.

Monte Carlo ray tracing program *designed* to simulate X-ray optical systems

68 / SPIE Vol. 503 Application, Theory, and Fabrication of Periodic Structures (1984)

Ray tracing of recent VUV monochromator designs

F. Cerrina

Department of Electrical and Computer Engineering
University of Wisconsin, Madison WI 53706

Abstract

A new optical ray-tracing program is presented and some applications discussed. A Monte-Carlo modelling of several types of sources is implemented, and in particular the Synchrotron Radiation source is modelled exactly. The program is written specifically for grazing optics, although gaussian optics can be treated as well. Diffraction from gratings, both ruled and holographic, is included as well as Bragg diffraction from crystals. The reflectivity of mirror surfaces and transmission of filters is treated exactly and locally, solving the Fresnel equations for each ray. The interactive nature of the program and its fast execution time allow the simulation of real-life situations quickly and efficiently. Applications to the Toroidal Grating Monochromator (TMG), Grating Crystal Monochromator (GCM), and Extended Range Grasshopper (ERG) are presented.

1990 SHADOW2 THE SWITCH TO UNIX

Large vision: from particular to generic

Freely available (mail distribution in magnetic tapes),

Good support (one dedicated person to users support and doc)

Robust design (survived so many years!).

Paid by other projects.

Many Cerrina's students contributed.

SHADOW2

New machines enter in the scientific computing market (Unix workstations: Digital/Ultrix, Sun, HP, …)

UNIX version prepared by Mumit Khan. First version installed at ESRF (1991)

Source opened

1988-1991 CRYSTALS: ASYMMETRIC, LAUE,

Asymmetrically cut crystals for synchrotron radiation monochromators

M. Sánchez del Río
European Synchrotron Radiation Facility, B.P. 220, 38043 Grenoble Cedex, France

F. Cerrina
Center for X-ray Lithography, 3731 Schneider Drive, Stoughton, Wisconsin 53589

(Presented on 22 July 1991)

936 Rev. Sci. Instrum. 63 (1), January 1992 0034-6748/92/010936-05$02.00 © 1992 American Institute of Physics 936

Nuclear Instruments and Methods in Physics Research A 347 (1994) 338–343
North-Holland

INSTRUMENTS & METHODS IN PHYSICS RESEARCH
Section A

Modeling perfect crystals in transmission geometry for synchrotron radiation monochromator design

M. Sánchez del Río [a,*], C. Ferrero [a], G-J. Chen [b], F. Cerrina [b]

[a] *European Synchrotron Radiation Facility, BP 220, 30043 Grenoble Cedex, France*
[b] *Center for X-ray Lithography, 3731 Schneider Drive, Stoughton, WI 53589, USA*

Focusing characteristics of diamond crystal x-ray monochromators. An experimental and theoretical comparison [a)]

M. Sánchez del Río and G. Grübel
European Synchrotron Radiation Facility, BP220 38043 Grenoble Cedex 9, France

J. Als-Nielsen
European Synchrotron Radiation Facility, BP220 38043 Grenoble Cedex 9, France and Risö National Laboratory, Roskilde, Denmark

M. Nielsen
Risö National Laboratory, Roskilde, Denmark

(Received 21 July 1994; accepted for publication 18 August 1995)

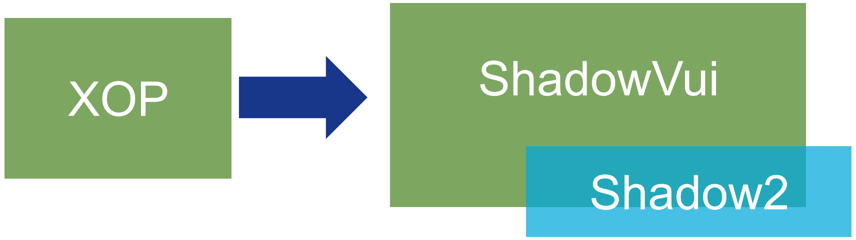
ELSEVIER

Nuclear Instruments and Methods in Physics Research B 94 (1994) 306–318

Beam Interactions with Materials & Atoms

Multiple station beamline at an undulator X-ray source

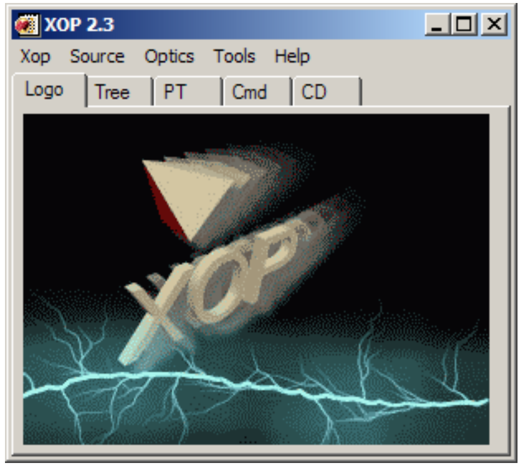
J. Als-Nielsen [a,b,*], A.K. Freund [b], G. Grübel [b], J. Linderholm [a,b], M. Nielsen [a],
M. Sanchez del Rio [b], J.P.F. Sellschop [c]

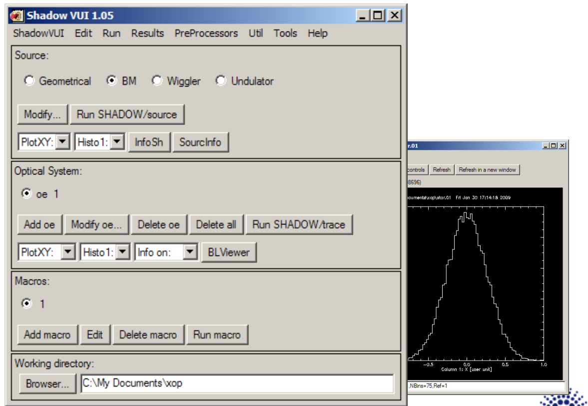


- IDL technology
- Communications via files

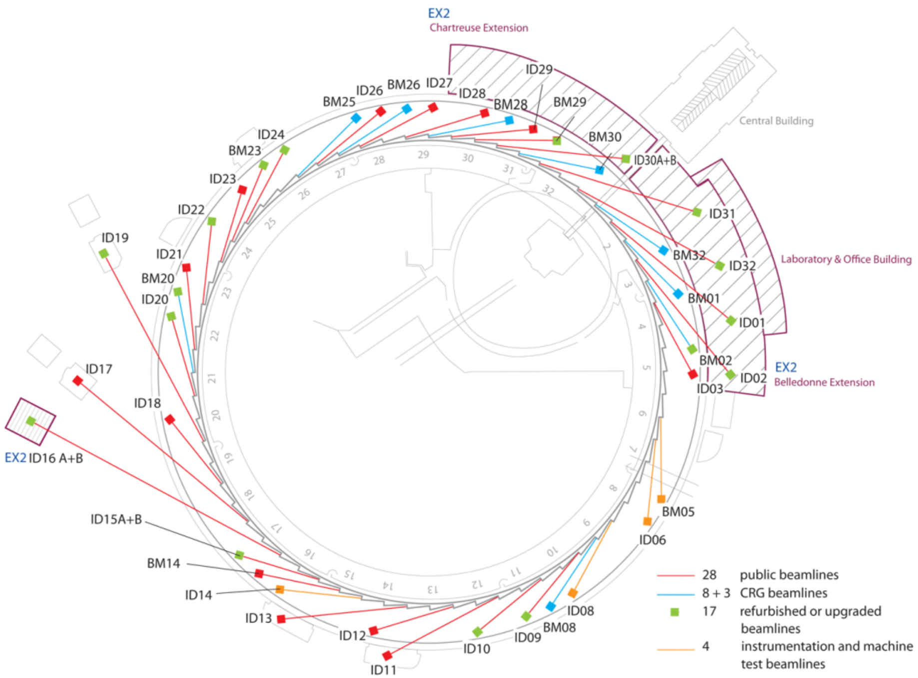
- ShadowVUI: interface that uses the standard SHADOW calculation engine
    - “Easy” to use
    - High performance graphics
    - Macro language
    - Tutorials
    - BLViewer
- XOP
    - quick calculations (synchrotron spectra, reflectivities, rocking curves, attenuation coeffs. etc.)
    - generic data visualization and analysis
    - specific applications (“extensions”)

    - Collaboration with APS (Roger Dejus)
    - Freely available to users (>10 years)
    - Large user community (>400 users in tens of laboratories)
    - Multiplatform (Windows, Unix, MacOSX)
    - Written in IDL (using Fortran and C modules). Embedded license.





PHASE I - 2008 - UPGRADE BEAMLINES



- ~1998-2007 Hiatus: Data analysis. XOP +SHADOW maintenance
- 2008-2009:
  - Launch of ESRF Upgrade
  - Creation of ISDD
  - I was fully assign to optics simulations

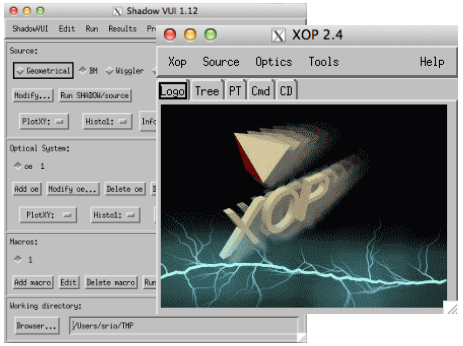
		From	To
UPBL1	Diffraction imaging for nano analysis	ID01	ID01
UPBL2	High energy beamline for buried interface structures and materials processing	ID15	ID31
UPBL4	Nano-imaging and nano-analysis	ID22	ID16
UPBL6	Inelastic hard X-ray scattering for electronic spectroscopy	ID16	ID20
UPBL7	Soft X-rays for magnetic and electronic spectroscopy	ID08	ID32
UPBL9A UPBL9B	• Time-resolved ultra small angle X-ray scattering • Pump-probe and time resolved experiments	ID02/ID09B	ID02/ID09
UPBL10	Massively automated sample selection integrated facility for macromolecular crystallography	ID14	ID30/BM29
UPBL11	Time resolved and extreme conditions X-ray absoption spectroscopy	ID24/BM29	ID24/BM23

TOWARDS SHADOW3

- ESRF Upgrade. Implications
  - Long beamlines: a few o.e., high demagnification, increased coherence
  - New trends: nanofocusing, partial coherence
  - New optics: CRL, transfocators, etc.

- Actions for modeling:
  - New tools? Other solutions examined. Stay on reliable solution
  - Renewal of SHADOW = shadow3
    - Contacts and visits to Cerrina (2008-2010)
    - Finish and maintain shadow3 at ESRF (since 2010)
  - Need of complementarity (other codes)
  - Setting collaborations
  - Software development programme

SHADOW3 *http://forge.epn-campus.eu/projects/shadow3*



Scripts, GUI…

```
import Shadow
beam = Shadow.Beam()
src = Shadow.Source()
oe1 = Shadow.OE()
…
beam.genSource(src)
beam.traceOE(oe1,1)
…
```

OASYS

shadow3 (main)

shadow3 (kernel)

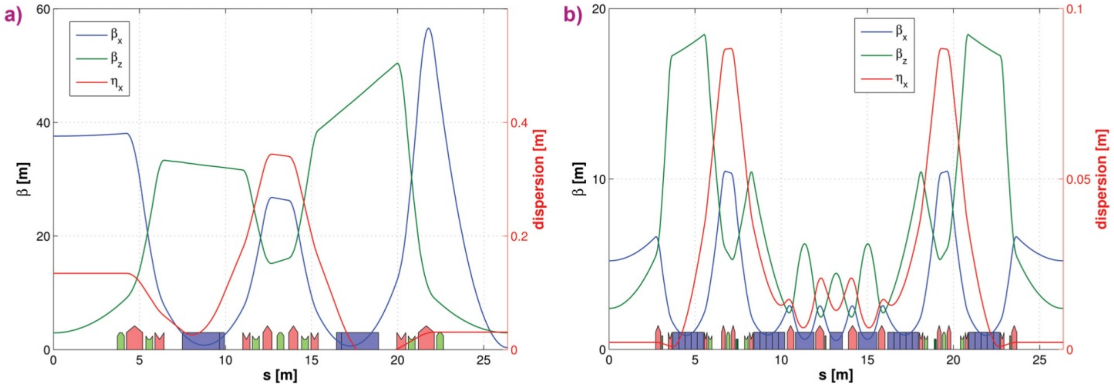
Preprocessors (optics library)

Postprocessors (graphics, etc)

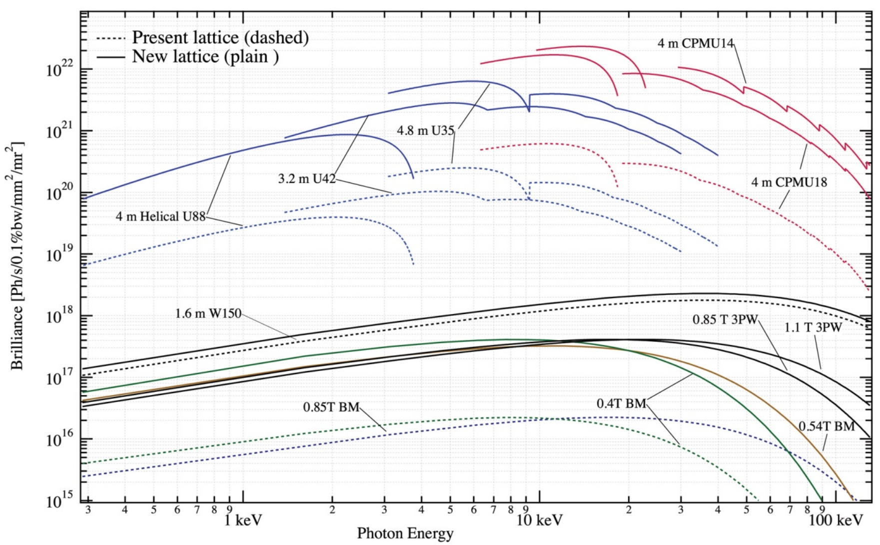
C

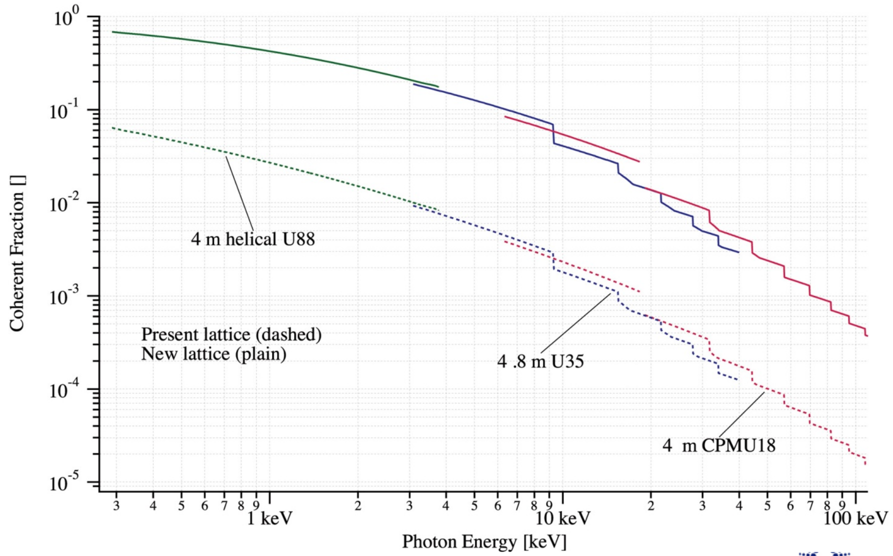
python

ESRF Upgrade Programme II =
ESRF EBS (Extremely Brilliant Source)



	Present lattice	New lattice
Lattice type	DBA	HMBA
Circumference [m]	844.390	843.979
Beam Energy [GeV]	6.04	6
Beam Current [mA]	200	200
Natural emittance [pm·rad]	4000	147
Energy spread [%]	0.106	0.095





MISSIONS

Fullfil ESRF needs for simulations of optics for Upgrade Phase I and transition to Phase II

Prepare scenario for optics calculations (and more) for Upgrade Phase II

Maintain present and define and implement further develop tools:

- -shadow3 maintenance and further development
- -migration obsolete technologies (IDL) to open source based tools (python)
- -complementary packages

Define and implement a new software infrastructure (OASYS)

Integration of software packages in it

Develop new complementary tools (HYBRID, DABAM, CRYSTAL,)

Look into coherence – Interest for SRW

Better understanding of partial coherence – Mark

Research: use tools for proposing new beamlines and optics concepts

Implementation and support of new tools for general users

GOAL: VIRTUAL EXPERIMETS – SOFTWARE INTEGRATION

Beamline Experiment Chain

Storage Ring (e^- optics) → Radiation devices (e^- -> γ) → Beamline (γ optics) → Sample (γ −matter interactions)

NEW OASYS-BASED TOOLBOX

ShadowOui

XPD

SRW

XOPpy

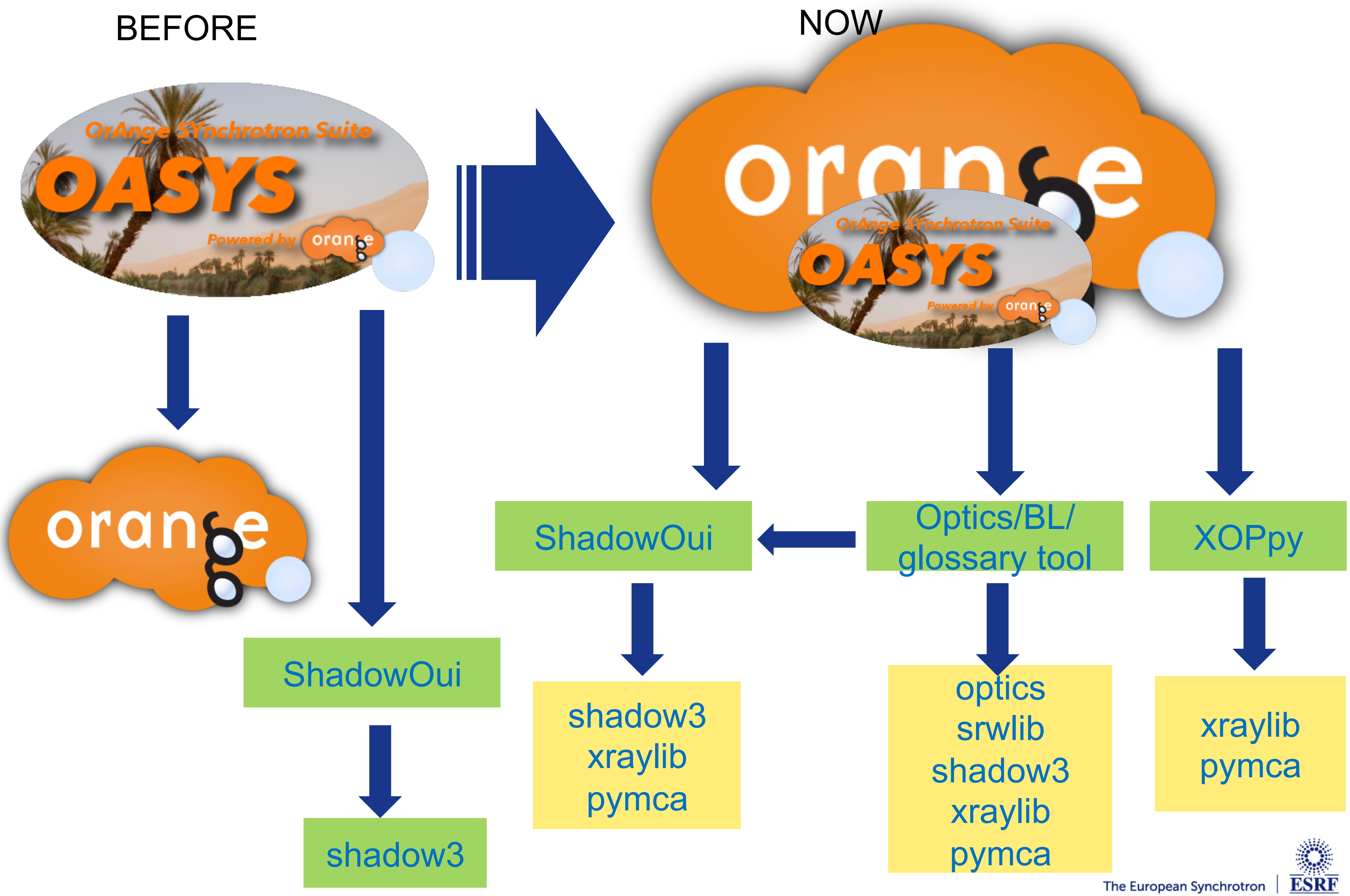
At-Collab

OTHER

WHAT IS ORANGE?

- Open Source project for Data Analysis and Visualization
- Developed in academic world (University of Ljubliana, Faculty of Informatics)
- Applied for data mining. We use the data workflow paradigma and replaced their widgets and flux (data) by our components and beams (rays, photons)
- Fully written in python (numpy, pyQt4, scipy, …)
- Intuitive and powerful box-based interface (workflow)
- The developers are nice and helpful, it is easy to work with them

OASYSIS ORANGE SYNCHROTRON SUITE (OASYS)



WHAT INFLUENCES THE PERFORMANCES OF A BEAMLINE

Photon source | Optics | Stability

Size
Divergence
Spectrum

Correlations

Emittance

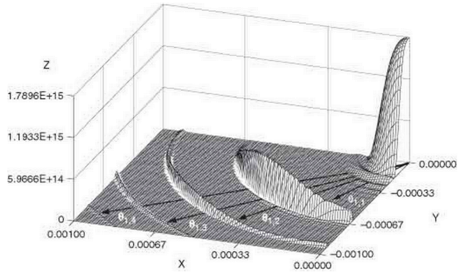
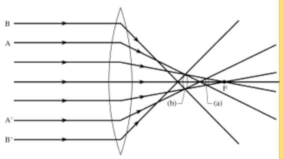
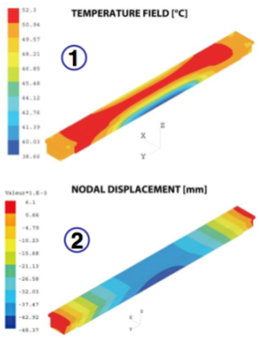
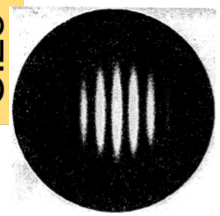
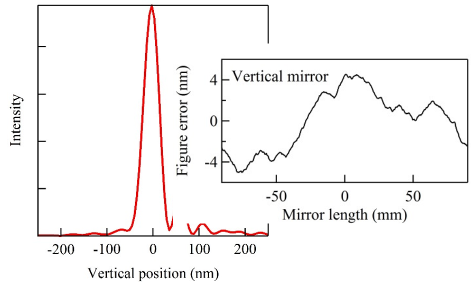


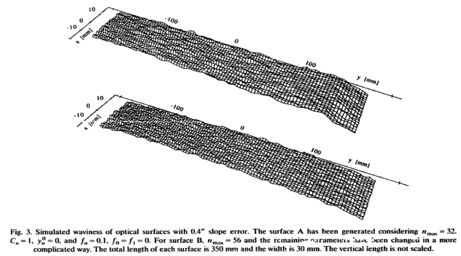
Figure (aberrations)
Figure (thermal & mechanical)
Slope errors
Roughness
Size (aperture)







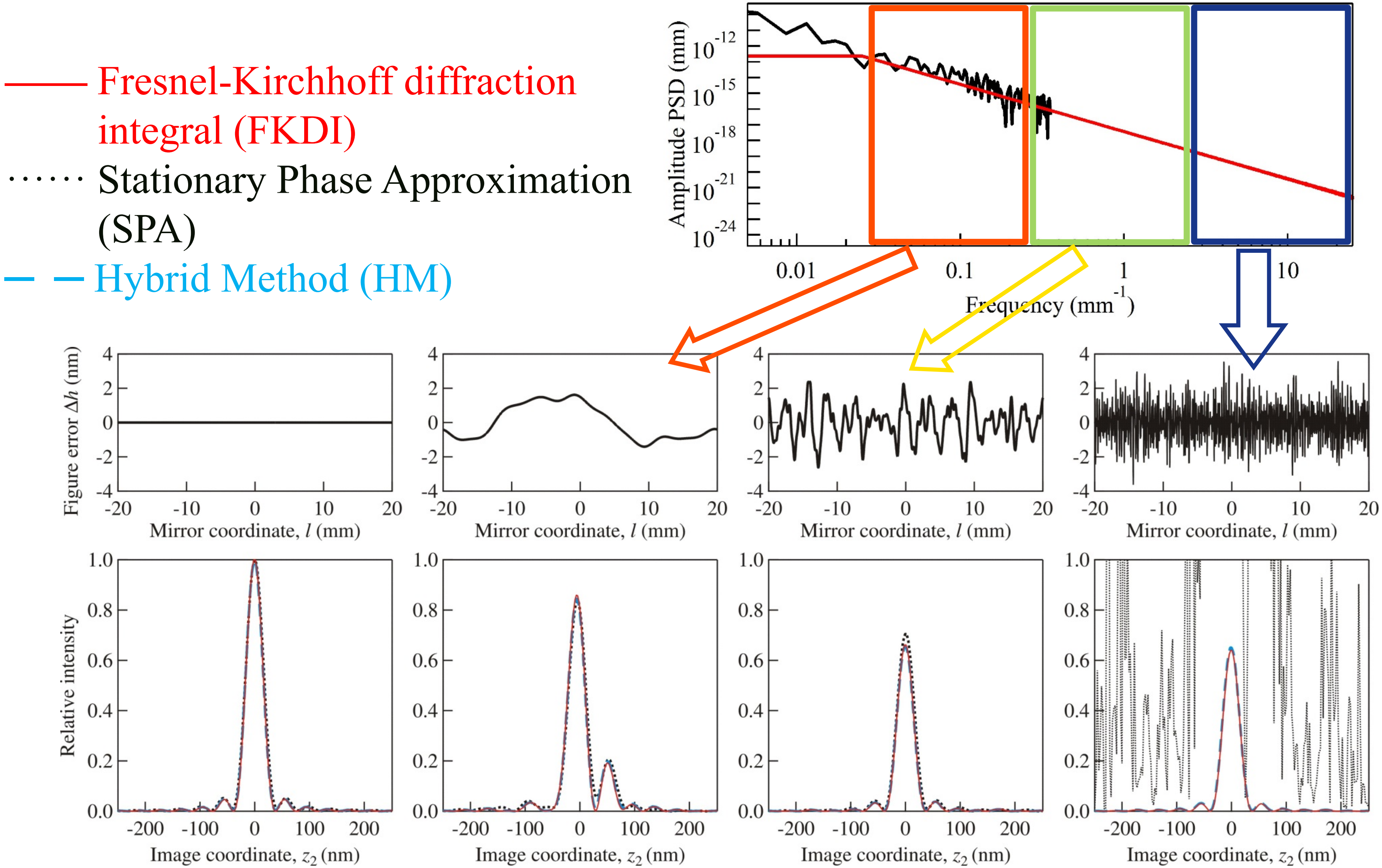




Temporal
Thermal
Mechanical

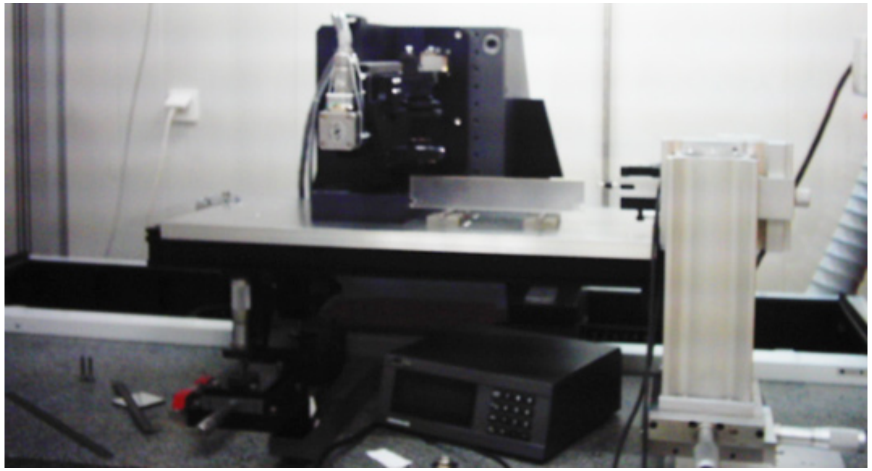
Correlations

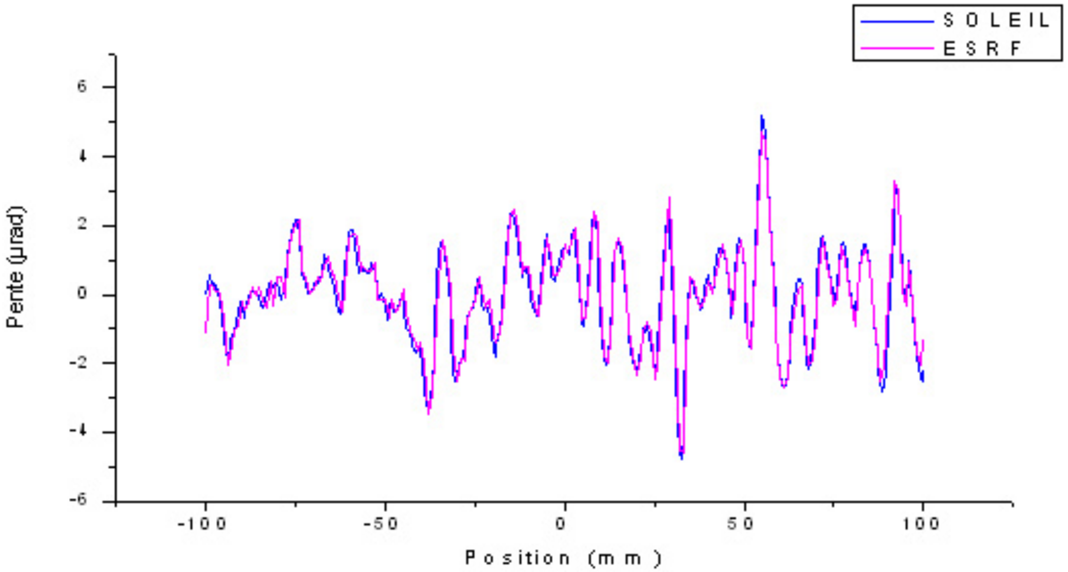
BEAM COHERENCE AND SURFACE ERRORS (XIANBO)



X. Shi, et al., Proc. SPIE **9209**, 920909 (2014).

DABAM: DATABASE FOR METROLOGY: MOTIVATION





This is not noise

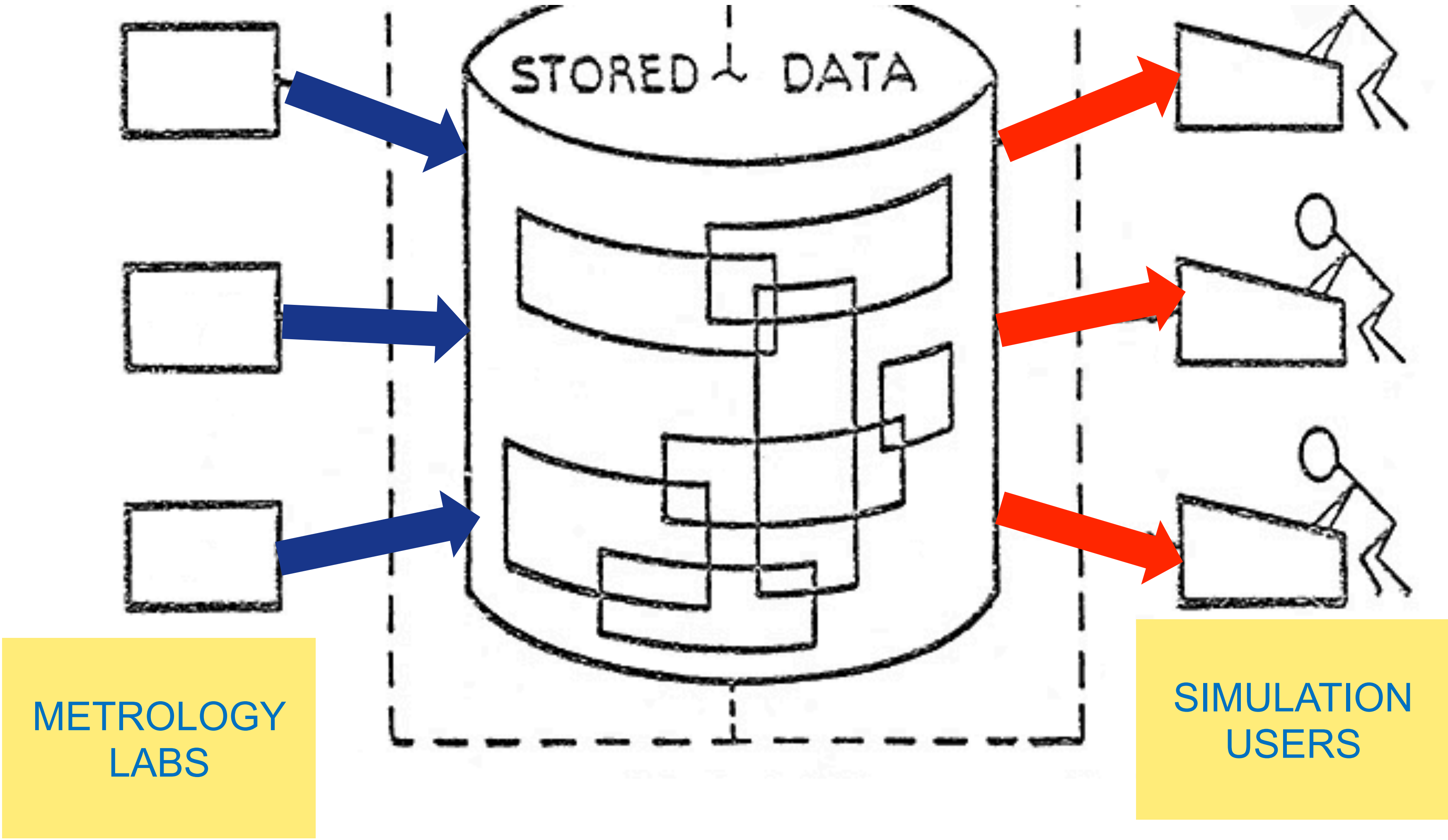
We can simulate “noisy” mirrors, but it is not the same

The best for simulations is to use real profiles

How to get them? Improve communication between metrology and simulation people

http://www.synchrotron-soleil.fr/Soleil/ToutesActualites/2010/Procedure-d-Elimination-des-Erreurs-de-Linearite

DABAM: DATABASE FOR METROLOGY



Repository with data (dabam-n.dat) and metadata (dabam-n.txt)
Python script to access and process data

ftp://ftp.esrf.eu/pub/scisoft/dabam/data/

Index of /pub/scisoft/dabam/data/

Name	Size	Date Modified
[parent directory]		
dabam-1.dat	14.6 kB	11/26/14, 12:00:00 AM
dabam-1.txt	662 B	11/26/14, 12:00:00 AM
dabam-10.dat	16.1 kB	11/26/14, 12:00:00 AM
dabam-10.txt	933 B	11/26/14, 12:00:00 AM
dabam-11.dat	16.1 kB	11/26/14, 12:00:00 AM

ftp://ftp.esrf.eu/pub/scisoft/dabam/data/dabam-12.dat

```
X(mm)   Measured heigth (nm)   Residual Heigth (nm)   Slope (micror-rad)   Resic
(microrad)
-221.0  175.6   -1.5    -3.4    -1.77579
-220.0  172.2   -3.3    -2.55   -0.933182
-219.0  170.5   -3.4    -1.85   -0.240575
-218.0  168.5   -3.8    -1.25   0.352032
-217.0  168.0   -2.7    -1.65   -0.0553617
-216.0  165.2   -3.9    -1.9    -0.312755
```


```
{
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  "POLISHING": null,
```

$ python3 dabam.py 11

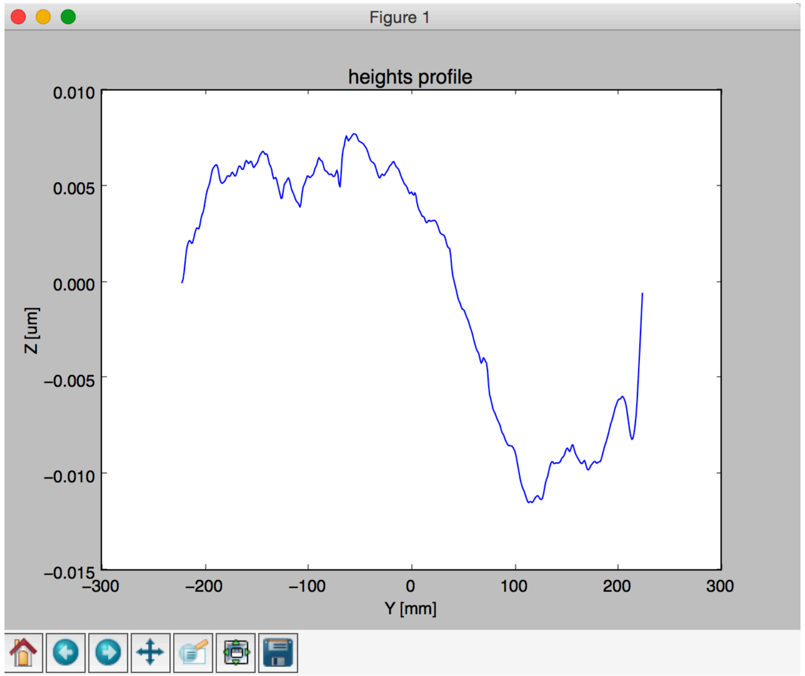
Using: abscissas column index 0 (mirror coordinates)
ordinates column index 1 (profile heights)
File tmpHeights.dat written to disk: Columns are:
coordinate(m),height(m).
File tmpSlopes.dat written to disk: Columns are:
coordinate(m),slopes(rad).
File tmpPSD.dat written to disk: Columns are:
freq (m^-1),psd_prof(m^3),psd_slope(rad^3),
cdf(psd_prof),cdf(psd_slope).

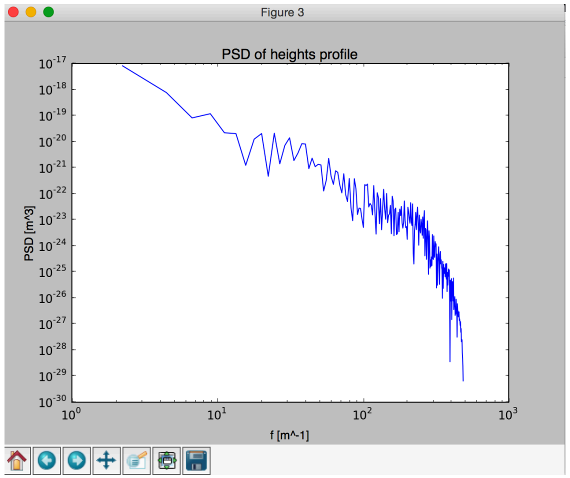
---------- profile results --------------------
Remote directory:
http://ftp.esrf.eu/pub/scisoft/dabam/data/
Data File: dabam-11.dat
Metadata File: dabam-11.txt
Surface shape: plane
Facility: LCLS
Scan length: 445.740 mm
Number of points: 438

Linear detrending: z'=1.34729e-06 x+5.74225e-08
Radius of curvature: 742231.253 m

Slope error s_RMS: 0.229 urad
from PSD: 0.156 urad
from USER (metadata): 0.2290927 urad
Shape error h_RMS: 6.582 nm
from PSD: 3.489 nm
from USER (metadata): 3.23343 nm
PV of height profile (before detrend): 43.942 nm
PV of height profile (after detrend): 19.216 nm
----

python3 dabam.py 11 -P heights -s --shadowNy 300 --shadowNx 20





SHADOW3 ACTIVITY

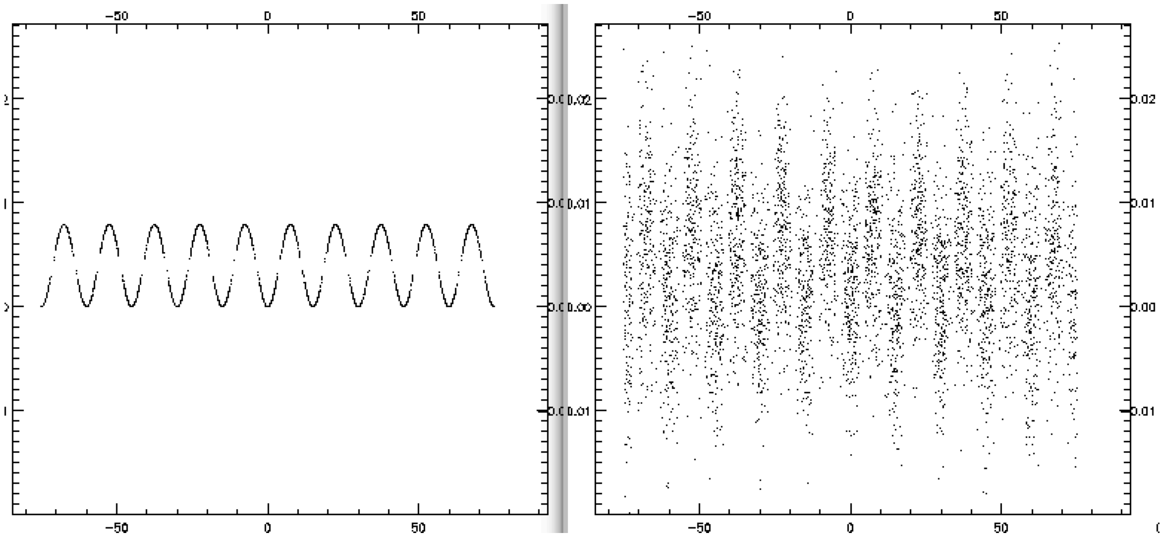
Python tools

- update of the python tools – coordinate with Oasys
- preprocessors (using xraylib)
- postprocessors (pre-graphics)
- compound elements (CRL, transfocators, DCM)
- installation (pypi thanks to RADIASOFT)

Sources:

- check models and update: wiggler, undulator (on going)
- Improve models for emittance (on going)

Others



PARTIAL COHERENCE (M GLASS)

Fully incoherent

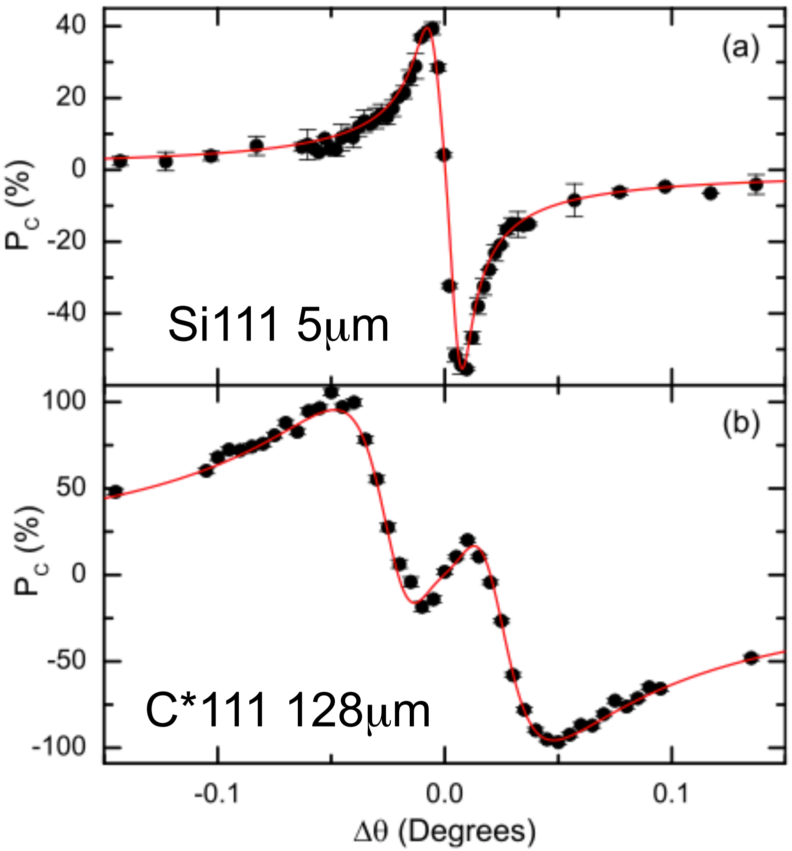
Partial coherence:

- Multi-e- (sum the emission of single e^-)
- Hybrid models
- Coherence degree of sources (undulators)
- Statistical Optics
- Gauss-Schell beams (coherent-mode decomposition)
- Wigner optics
- …

Fully coherent

Bouchenoire, Morris, Hase

Appl. Phys. Lett. **101**, 064107 (2012)



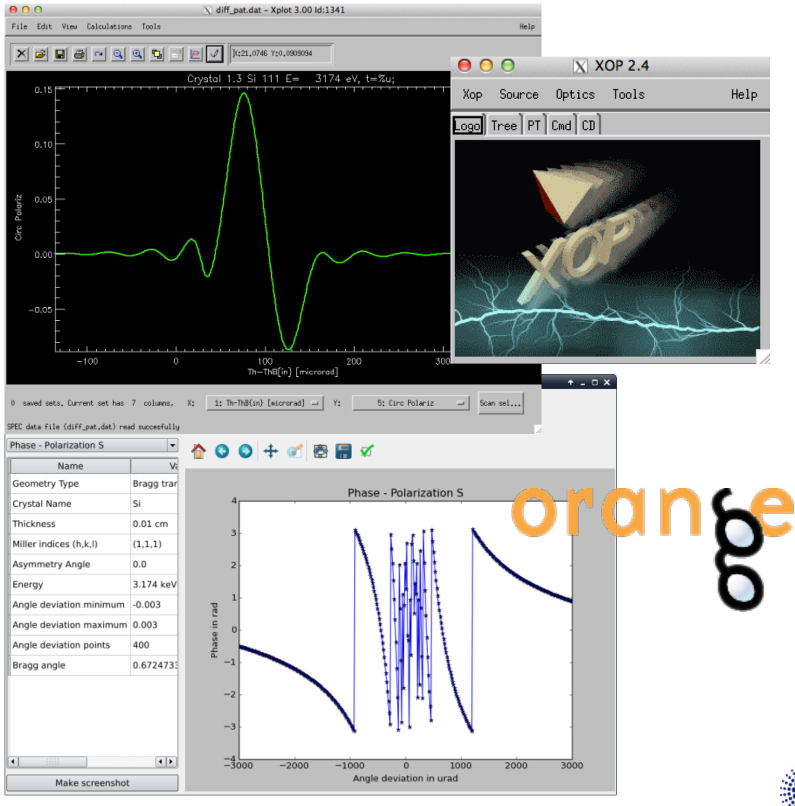
E=3.174 keV

$$\begin{pmatrix} E_x(t) \\ E_y(t) \end{pmatrix} = E^{(0)} \exp[i(-\omega t + \phi_x)] \begin{pmatrix} V_x \\ V_y \end{pmatrix},$$

Jones Matrices

$$\mathbf{R} = \begin{pmatrix} R_\sigma & 0 \\ 0 & R_\pi \end{pmatrix}$$

$$\mathbf{T} = \begin{pmatrix} T_\sigma & 0 \\ 0 & T_\pi \end{pmatrix} = \begin{pmatrix} t_\sigma e^{i\phi_\sigma} & 0 \\ 0 & t_\pi e^{i\phi_\pi} \end{pmatrix}$$



STOKES-MUELLER CRYSTAL OPTICS (M GLASS)

Stokes parameters

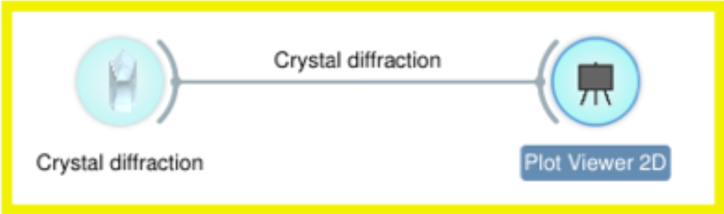
$$
\begin{aligned}
I &\equiv |E_x|^2 + |E_y|^2 \quad (= |E_a|^2 + |E_b|^2 = |E_l|^2 + |E_r|^2) \\
Q &\equiv |E_x|^2 - |E_y|^2 \\
U &\equiv |E_a|^2 - |E_b|^2 \\
V &\equiv |E_l|^2 - |E_r|^2
\end{aligned}
$$

Mueller Matrices

$$
M_{\mathrm{PP}} = \begin{pmatrix} t_\sigma e^{i\phi_\sigma} & 0 \\ 0 & t_\pi e^{i\phi_\pi} \end{pmatrix}
$$

$$
\mathcal{M}_{\mathrm{PP}} = \begin{pmatrix} t_\sigma^2 + t_\pi^2 & t_\sigma^2 - t_\pi^2 & 0 & 0 \\ t_\sigma^2 - t_\pi^2 & t_\sigma^2 + t_\pi^2 & 0 & 0 \\ 0 & 0 & t_\sigma t_\pi \cos(\Delta\phi) & -t_\sigma t_\pi \sin(\Delta\phi) \\ 0 & 0 & t_\sigma t_\pi \sin(\Delta\phi) & t_\sigma t_\pi \cos(\Delta\phi) \end{pmatrix}
\qquad
\mathcal{M}_{j,i} = \frac{1}{2}\mathrm{tr}(\boldsymbol{\sigma}_i \cdot \mathbf{M} \cdot \boldsymbol{\sigma}_j \cdot \mathbf{M}^\dagger).
$$

$$
\begin{aligned}
I' &= \frac{I}{2}\left[t_\sigma^2 + t_\pi^2 + P_1(t_\sigma^2 - t_\pi^2)\right] \\
&\approx I t^2 \left(1 + \tau P_1\right) \\
P_1' &= \frac{t_\sigma^2 - t_\pi^2 + P_1(t_\sigma^2 + t_\pi^2)}{t_\sigma^2 + t_\pi^2 + P_1(t_\sigma^2 - t_\pi^2)} \\
&\approx P_1 + \tau\left(1 - P_1^2\right) \\
P_2' &= \frac{2 t_\sigma t_\pi \left[\cos(\Delta\phi) P_2 - \sin(\Delta\phi) P_3\right]}{t_\sigma^2 + t_\pi^2 + P_1(t_\sigma^2 - t_\pi^2)} \\
&\approx \left[\cos(\Delta\phi) P_2 - \sin(\Delta\phi) P_3\right]\left(1 - \tau P_1\right) \\
P_3' &= \frac{2 t_\sigma t_\pi \left[\sin(\Delta\phi) P_2 + \cos(\Delta\phi) P_3\right]}{t_\sigma^2 + t_\pi^2 + P_1(t_\sigma^2 - t_\pi^2)} \\
&\approx \left[\sin(\Delta\phi) P_2 + \cos(\Delta\phi) P_3\right]\left(1 - \tau P_1\right),
\end{aligned}
$$



C Detlefs, M Sanchez del Rio, C Mazzoli Eur. Phys. J. Special Topics 208, 359–371 (2012)

PRL 97, 235502 (2006) PHYSICAL REVIEW LETTERS week ending 8 DECEMBER 2006

X-Ray Bragg Diffraction in Asymmetric Backscattering Geometry

Yu. V. Shvyd'ko*
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M. Lerche
University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA
Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA

U. Kuetgens
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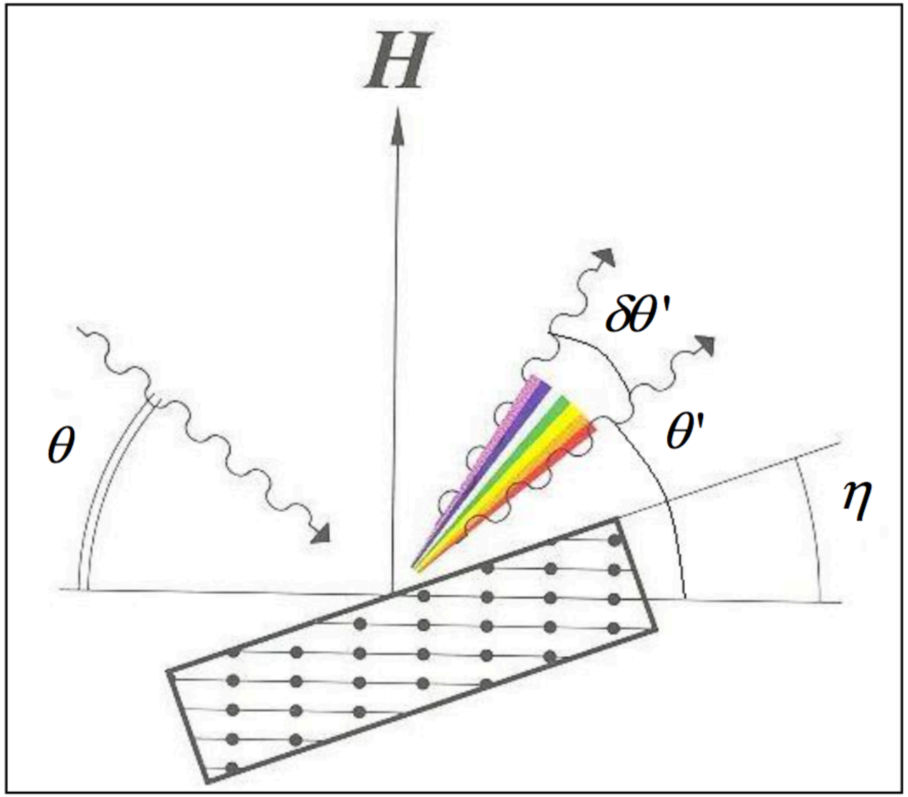
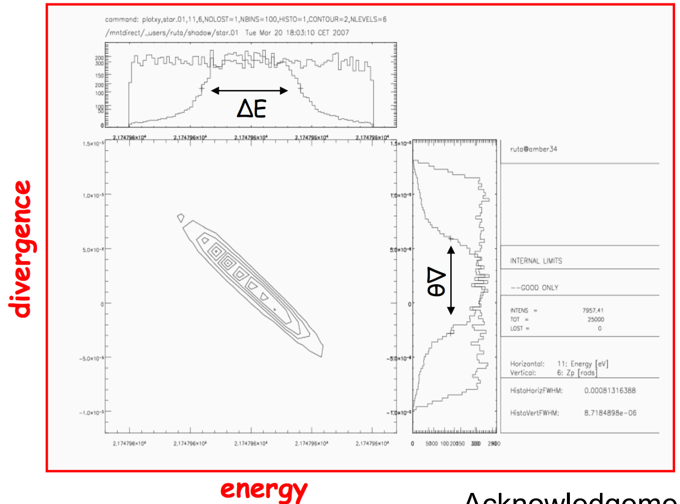
H. D. Rüter



$$\delta\theta' = 2\frac{\delta E}{E}\tan\eta$$

Beam after the reflection from Si(11,11,11) monochromator with η= 89.5°.



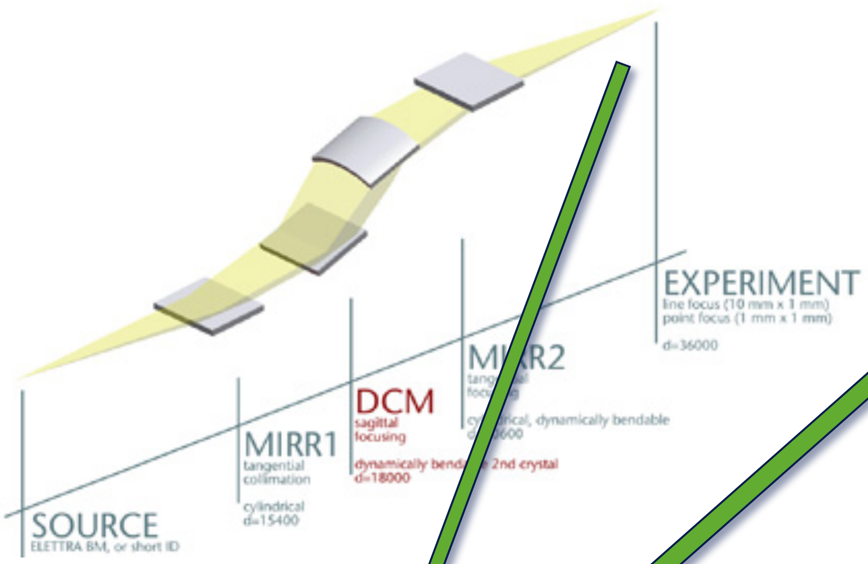
ΔE=0.8 meV

Δθ=8.7μrad

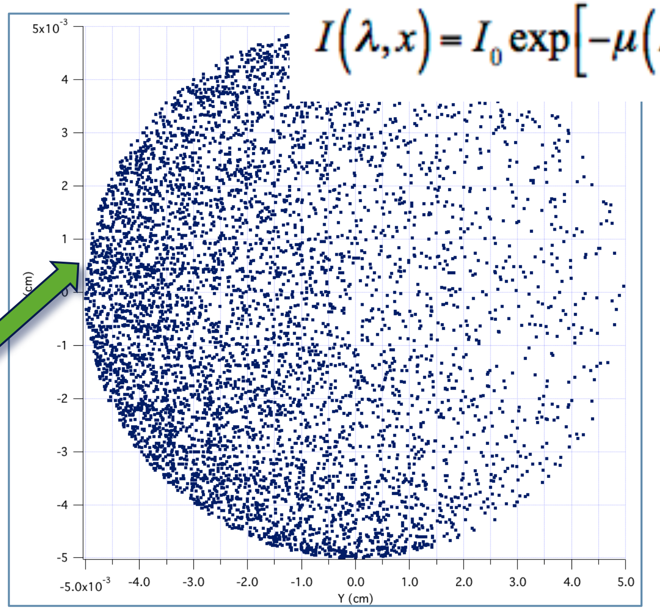
As expected from the theory!

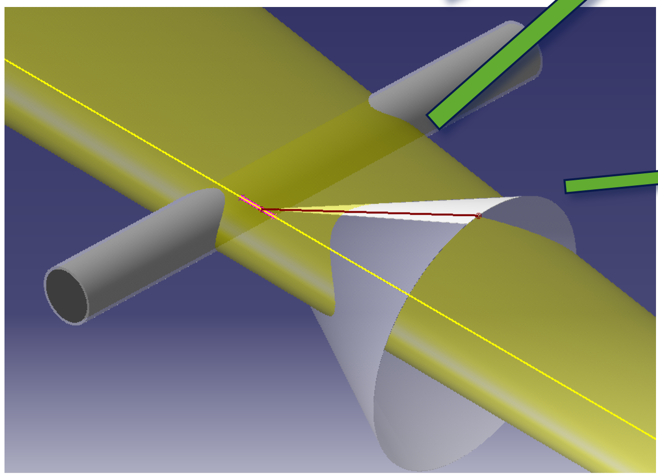
Acknowledgement: B Ruta

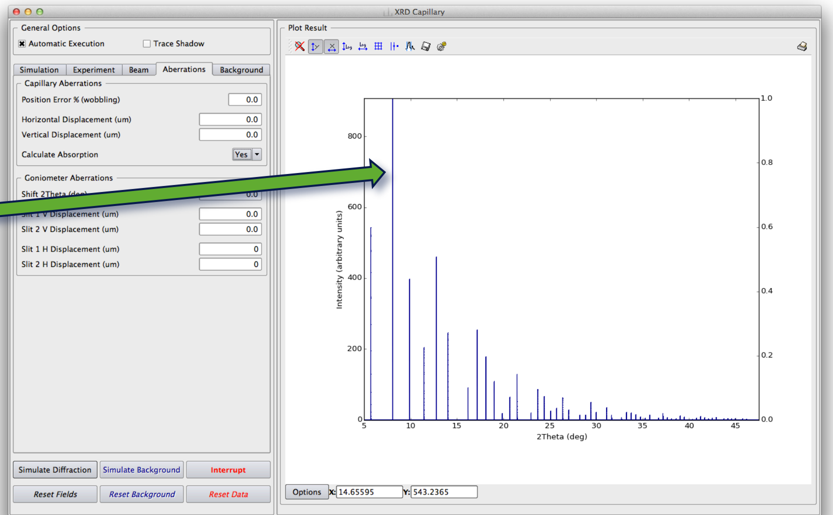
SAMPLE SIMULATIONS (LUCA)



$$I(\lambda, x) = I_0 \exp\left[-\mu(\lambda)\rho x\right]$$







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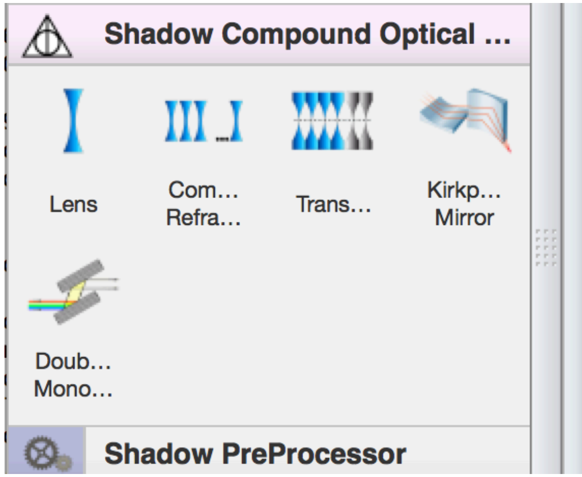
Integration in ShadowOui

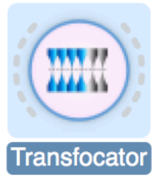
Quick search for configuration (ID30B)

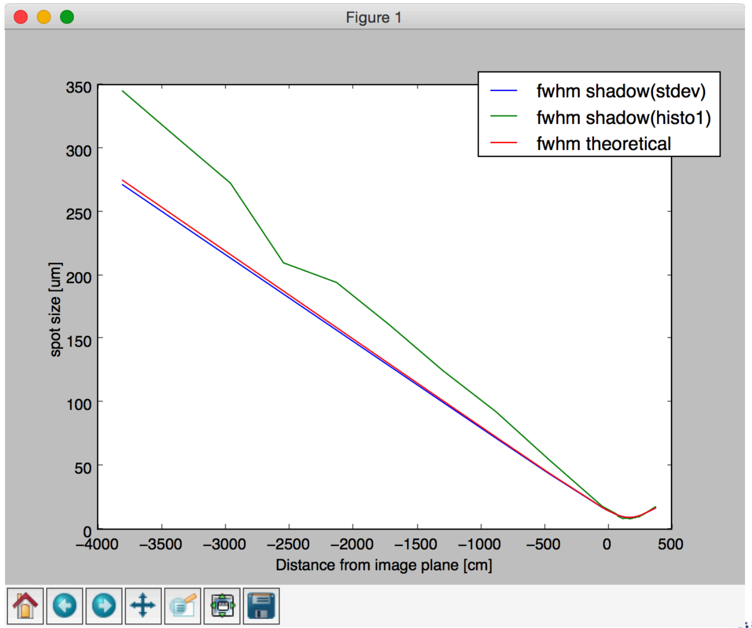
Quick calculations

Standarization

```
Manuels-MacBook-Pro:tmp srio$ python3 ~/xop2.4/extensions/shadowvui/python_scripts/
transfocator_id30b.py
Enter:
  0 = optimization calculation only
  1 = full simulation (ray tracing)
?> 1
Enter photon energy in keV: 20
Enter target focal dimension in microns: 20
================================= TRANSFOCATOR INPUTS
Photon energy: 20000.000000 eV
target size: 0.002000 cm
materials:  ['Be', 'Be', 'Be']
densities:  [1.845, 1.845, 1.845]
Lens diameter: 0.050000 cm
nlenses_max: [15, 3, 1] nlenses_radii:  [0.05, 0.1, 0.15]
Source size (sigma): 6.460000 um, FWHM: 15.181000 um
Distances: tf_p: 5960.000000 cm, tf_q: 3800.000000 cm
alpha: 0.550000
=======================================================
transfocator_compute_configuration: focal_f_target: 2412.252318
transfocator_compute_configuration: focal_q_target: 4052.436954 cm
transfocator_compute_configuration: s_target: 20.000000 um
transfocator_compute_configuration: nlenses_target:  [11, 2, 1]
============================== TRANSFOCATOR SET
nlenses_target (optimized):  [11, 2, 1]
With these lenses we obtain:
  focal_f: 2384.195960 cm
  focal_q: 3973.877697 cm
  s_target: 15.723904 um
  slots_max:     [1, 2, 4, 8, 1, 2, 1]
  slots_on_off:  [1, 1, 0, 1, 0, 1, 1]
=================================================
Start SHADOW simulation? [1=yes,0=No]: 1
```







LENSES: ABERRATION-FREE SINGLE LENSE

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Aspherical lens shapes for focusing synchrotron beams

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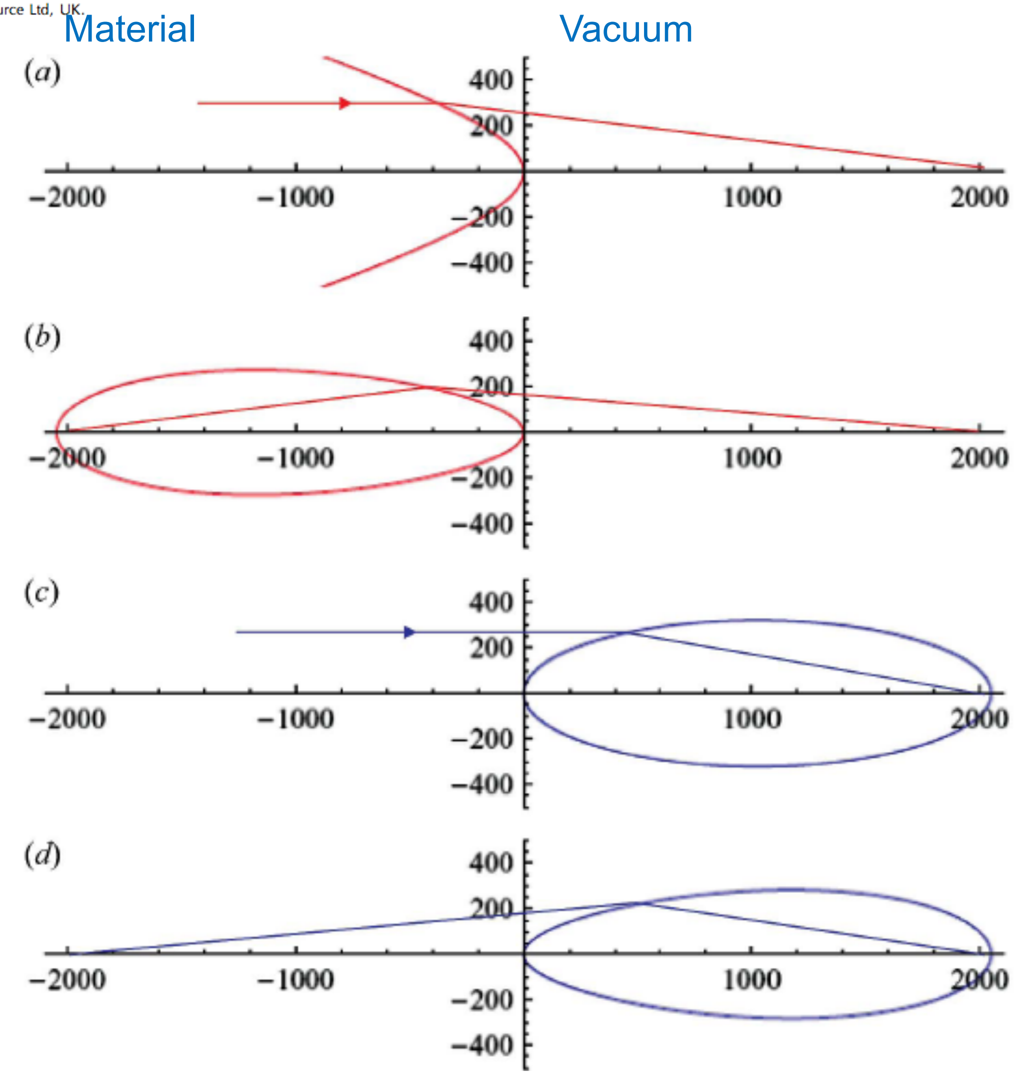
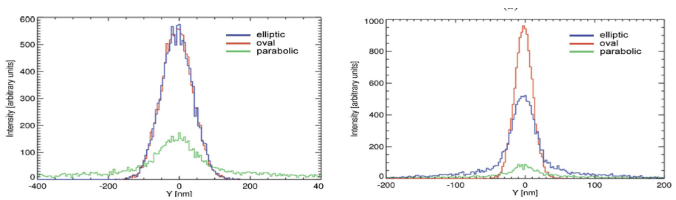
	$n_1 < n_2$	$n_1 > n_2$
Collimated to convergent	Ellipse c)	Hyperbola a)
Convergent to collimated	Hyperbola	Ellipse
Divergent to convergent	Cartesian oval d)	Cartesian oval b)

Figure 4
Ideal surface shape for different focusing conditions.

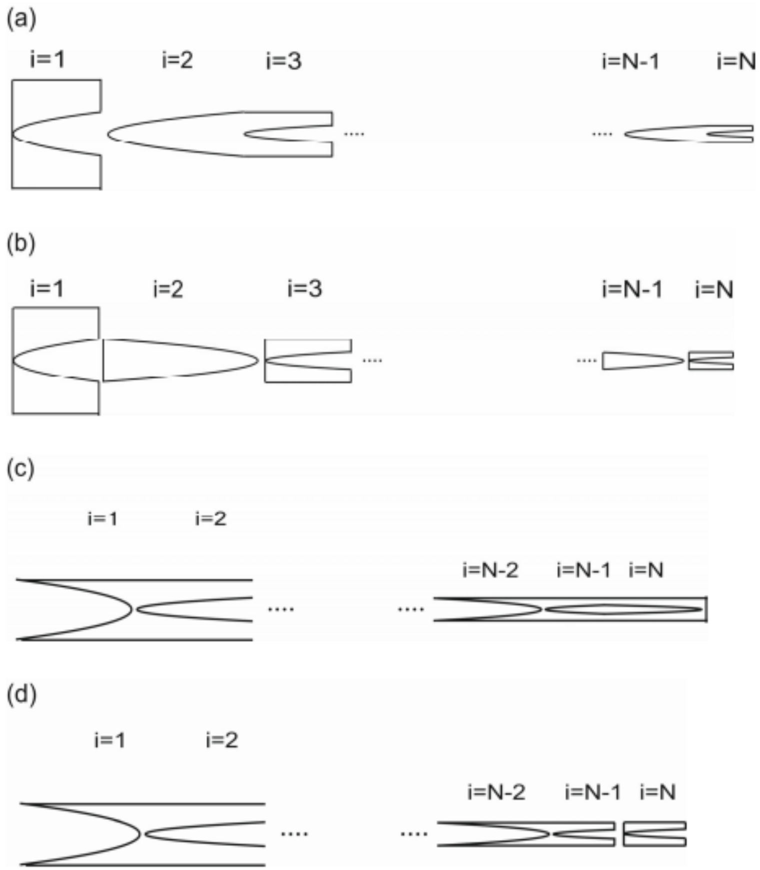




E=8 keV; Si Lens; p=47 m; *h*=0.3 mm
q=30 cm
M=157

q=10 cm
M=470

LENSES: ABERRATION-FREE SYSTEMS



Aberration-free short focal length x-ray lenses

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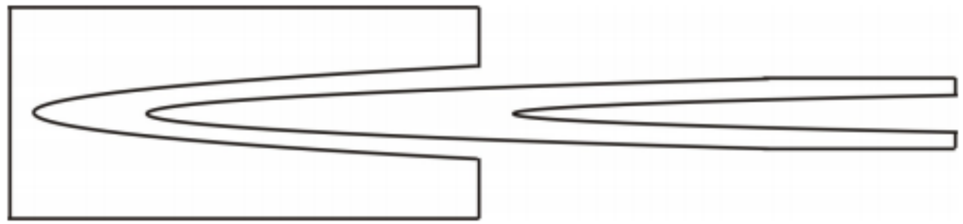
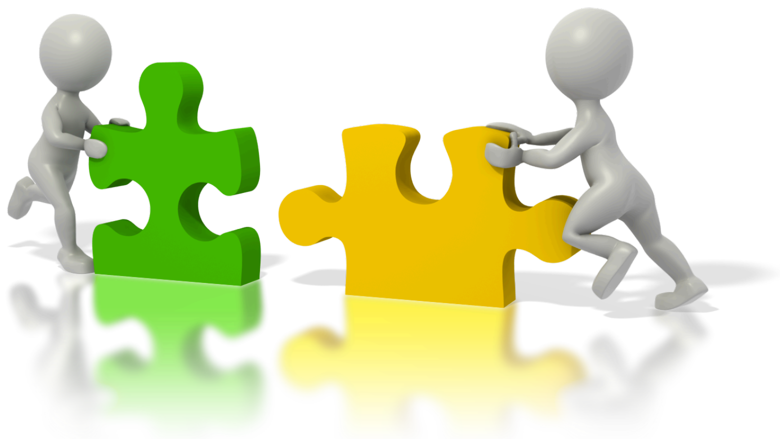
We treat the problem of defining the ideal x-ray refractive lens design for point focusing of low emittance x-ray beams at third- and fourth-generation synchrotron sources. The task is accomplished by using Fermat's principle to define a lens shape that is completely free from geometrical aberrations. Current micro-fabrication resolution limits are identified and a design that tolerates the inherent fabrication imperfections is proposed. The refractive lens design delivers nanometer-sized focused x-ray beams and is compatible with current micro-fabrication techniques.



(a) N elliptical surfaces;
(b) $N/2$ ellipses (for odd values of i) and $N/2$ hyperbolas (for even values of i);
(c) N hyperbolic surfaces;
(d) $N-1$ hyperbolic surfaces with a final elliptical surface.



Thanks!